

Low-Rank Approximation in Spectral Stochastic Finite Element Method with Solution Space Adaption

Informatikbericht 2010-03

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November 4, 2010

Abstract: *The Spectral Stochastic Finite Element Method (SSFEM) has become one of the most interesting methods in solving partial differential equations with stochastic parameters. In its classical form it underlies the Curse of Dimension. Many different techniques have been developed recently to go against that curse and consequently to make SSFEM applicable for high dimensional problems. These techniques include Low-Rank approaches and solution space reductions. We present a rank-one update scheme based on the variational formulation of the problem. The resulting Low-Rank representation is not necessarily an optimal one with respect to the minimum energy at the given rank. This scheme is extended to an optional solution space adaption and the possibility to compute an optimal decomposition.*

Keywords: *Spectral Stochastic Finite Element Method, Low-Rank approximation, successive rank-one update, residual-based solution space adaption*

Motivation

Many physical phenomena exhibit uncertain input. As a consequence their output becomes also uncertain. Such uncertainties can be observed e.g. in the flow through porous media caused by the involved heterogeneous ground. Similar circumstances occur in solid mechanics due to the heterogeneity of the considered material, e.g. concrete.

However the uncertainty is part of the phenomenon itself and need to be modelled for a reasonable numerical simulation to predict the behaviour of the considered problem. A stochastic description of the input and output allows a detailed uncertainty representation.

The Spectral Stochastic Finite Element Method (SSFEM) [6, 7, 4] has been considered with big interest, as it may offer better convergence characteristics as their opponents, the Monte Carlo and Quasi-Monte Carlo methods and Stochastic Collocation methods [1, 11, 12, 5] as well as straight forward projection methods based onto integration [9, 8].

The classical form of the SSFEM uses only two parameters to choose the solution space: the dimension and the order of the spanning basis functions. For instance properties of the numerical model itself are not taken into account. By using such a classical choice the size of the solution space grows exponentially when increasing the two mentioned parameters. This undesired property is known as the *Curse of Dimension* in the literature.

Low-Rank representations and adaptive solution space techniques have been developed recently for a practical applicability of the SSFEM. In [3] a Low-Rank approximation of the numerical problem to be considered is done on a geometrically coarse mesh to derive afterwards few basis functions to represent the solution efficiently. These basis functions are transferred to the geometrically fine discretised numerical problem to be solved actually. A spectral decomposition of the stochastic solution field is derived from the expectation of the minimum total potential energy principle in [14, 13]. This approach is referred to as the *Generalized Spectral Decomposition (GSD)* method. In this context three different numerical algorithms are presented to solve the resulting numerical system. In [10, 15] a Low-Rank representation of the solution field is directly substituted in the fully discretised stationary diffusion equation with stochastic parameter. Higher rank matrices arise due to the composition of the system matrix itself. This rank increase is reduced by applying a truncated *Singular Value Decomposition (SVD)*. This is done so to say “on the fly” meaning inside each iteration step of the numerical scheme to solve the problem. A solution space reduction in a preprocessing step is proposed in [2]. Here the geometrical degrees of freedom are virtually reduced to one. The resulting purely stochastic model – named “zero-dimensional model” – is used to extract the best basis functions (from a predefined set of basis functions) for the actual numerical problem to be solved.

In general the idea of a Low-Rank approximation is orthogonal to a solution space reduction. In contrast to [14, 13] we derive directly a rank-one update scheme from the minimum total potential energy principle. The resulting algorithm is comparable to a special form of the so called “restarting algorithm” of the GSD, see [14, 13]. However our algorithm in its standard form does not necessarily produce an optimal Low-Rank representation concerning the minimum energy at the given rank. We extend the algorithm to an optional adaptive solution space technique and a rank reduction technique to get an optimal Low-Rank decomposition.

Model

We consider the stationary groundwater flow equation (syntactically equal to the stationary diffusion equation)

$$(1) \quad \nabla_{\mathbf{x}} \kappa(\mathbf{x}, \omega) \nabla_{\mathbf{x}} u(\mathbf{x}, \omega) = f(\mathbf{x})$$

with the uncertain hydraulic head u and the uncertain hydraulic conductivity κ – each of both represented by a stochastic field defined onto the geometrical variable \mathbf{x} and the elementary event ω . The source term f and the boundary conditions (not specified explicitly here) are considered to be deterministic. κ is assumed to be non-Gaussian distributed and is available in a truncated *Karhunen-Loève Expansion (KLE)*, a spectral decomposition of the form $\kappa(\mathbf{x}, \omega) \approx \bar{\kappa}(\mathbf{x}) + \sum_{i=1}^m \sqrt{\lambda_i} \kappa_i(\mathbf{x}) \xi_i(\omega)$. $\bar{\kappa}$ is the expected value of κ . λ_i 's and κ_i 's are the i 'th largest eigenvalues and corresponding eigenfunctions of the Fredholm integral of the 2nd kind with the covariance function of κ as kernel. The random variables $\{\xi_i(\omega)\}_{i \in \{1, \dots, m\}}$ are uncorrelated, centered and of unit variance. These variables are discretised each by a truncated so called *Polynomial Chaos Expansion (PCE)* in orthogonal Hermite polynomials $\{\psi_\gamma\}_{\gamma \in \mathcal{I}}$ defined onto a Gaussian distributed random vector $\boldsymbol{\theta}$: $\xi_i(\omega) \approx \sum_{\alpha \in \mathcal{I}} \xi_{i,\alpha} \psi_\alpha(\boldsymbol{\theta})$.

Deriving the weak form of equation 1 and using truncated PCEs for the test and the ansatz functions as well as an analogous geometrical discretisation leads to the fully discretised system to be solved. It is given by

$$(2) \quad \sum_{i=0}^l \mathbf{K}_i \mathbf{U} \Delta_i = \mathbf{F} \quad \Longleftrightarrow \quad \mathcal{A}(\mathbf{U}) = \mathbf{F}$$

with $[\Delta_i]_{\alpha,\beta} := \sum_{\gamma \in \mathcal{I}} \sqrt{\lambda_i} \xi_{i,\gamma} [\Delta_\gamma]_{\alpha,\beta}$ and $[\Delta_\gamma]_{\alpha,\beta} := \langle \psi_\alpha \psi_\beta \psi_\gamma \rangle$. The triple product $\langle \psi_\alpha \psi_\beta \psi_\gamma \rangle$ marks the expected value of the product of the ansatz function ψ_α , the test function ψ_β and the basis function ψ_γ of the discretised parameter κ . \mathbf{K}_i is the stiffness matrix, in which the material parameter is declared as the i 'th eigenvector (FEM discretised eigenfunction) of the KLE of κ . We refer to [7] for more details.

Variational Low-Rank Approach with Successive Rank-One Update (VLR-SR1U)

We derive a SSFEM Low-Rank scheme with successive rank-one update from the expectation of the minimum total potential energy principle. For the fully discretised groundwater flow problem (see equation 2) this means to consider the minimisation problem:

$$(3) \quad \mathcal{E}(\mathbf{U}) := \frac{1}{2} \mathcal{A}(\mathbf{U}) : \mathbf{U} - \mathbf{F} : \mathbf{U} \longrightarrow \min.$$

This description is also identified as the variational formulation in the literature. The involved inner product $A : B := \sum_{i,j} A_{ij} B_{ij}$ with $A, B \in \mathbb{R}^{n_1 \times n_2}$ is the so called *Frobenius* one. We refer

the entire resulting scheme to as the *Variational Low-Rank Approach with Successive Rank-One Update* (VLR-SRIO). It corresponds to a special form of the restarting algorithm in [14, 13].

At this the ansatz

$$(4) \quad \mathbf{U} = \mathbf{U}^- + \mathbf{g}\mathbf{h}^T$$

describes the rank-one update of a given solution \mathbf{U}^- by the dyadic product of the geometrical update part \mathbf{g} and the stochastic update part \mathbf{h}^T . Differentiating the operator \mathcal{E} in equation 3 with respect to \mathbf{U} means

$$(5) \quad \frac{\partial \mathcal{E}(\mathbf{U})}{\partial \mathbf{U}}(\delta \mathbf{U}) = \underbrace{(\mathcal{A}(\mathbf{U}) - \mathbf{F})}_{=: R(\mathbf{U})} : \delta \mathbf{U}.$$

This allows to consider the perturbation of \mathbf{U} by varying once \mathbf{g} and once \mathbf{h} :

$$\begin{aligned} \frac{\partial \mathbf{U}}{\partial \mathbf{g}}(\delta \mathbf{g}) &= \delta \mathbf{g}\mathbf{h}^T \\ \frac{\partial \mathbf{U}}{\partial \mathbf{h}}(\delta \mathbf{h}) &= \mathbf{g}\delta \mathbf{h}^T. \end{aligned}$$

Then the derivatives of \mathcal{E} with respect to \mathbf{g} and \mathbf{h} are given by

$$(6) \quad \begin{aligned} \frac{\partial \mathcal{E}(\mathbf{U})}{\partial \mathbf{g}}(\delta \mathbf{g}) &= R_{\mathbf{U}} : (\delta \mathbf{g}\mathbf{h}^T) = \delta \mathbf{g}^T R_{\mathbf{U}} \mathbf{h} \\ \frac{\partial \mathcal{E}(\mathbf{U})}{\partial \mathbf{h}}(\delta \mathbf{h}) &= R_{\mathbf{U}} : (\mathbf{g}\delta \mathbf{h}^T) = \mathbf{g}^T R_{\mathbf{U}} \delta \mathbf{h} \end{aligned}$$

with $R_{\mathbf{U}} := R(\mathbf{U})$. The mentioned minimisation problem is expressed by $\frac{\partial \mathcal{E}(\mathbf{U})}{\partial \mathbf{g}}(\delta \mathbf{g}) \equiv 0$ and $\frac{\partial \mathcal{E}(\mathbf{U})}{\partial \mathbf{h}}(\delta \mathbf{h}) \equiv 0$. As $\delta \mathbf{g}$ and $\delta \mathbf{h}$ can be chosen arbitrarily, the following can be concluded:

$$(7) \quad \begin{aligned} R_{\mathbf{U}} \mathbf{h} &= \mathbf{0} \\ \mathbf{g}^T R_{\mathbf{U}} &= \mathbf{0}. \end{aligned}$$

Substituting \mathbf{U} by the iterative ansatz $\mathbf{U}_{r+1} = \mathbf{U}_r + \mathbf{g}_{r+1}\mathbf{h}_{r+1}^T$ with rank r , inserting this ansatz into the equations 7 and arranging them leads to the coupled system to be solved:

$$(8) \quad \begin{aligned} \mathcal{G} \mathbf{g}_{r+1} &= \mathbf{f} \quad \text{with} \quad \mathcal{G} := \sum_{i=0}^l \underbrace{\mathbf{h}_{r+1}^T \Delta_i \mathbf{h}_{r+1}}_{=: d_i} \mathbf{K}_i, \quad \mathbf{f} := (\mathbf{F} - \mathcal{A}(\mathbf{U}_r)) \mathbf{h}_{r+1}, \\ \mathcal{H} \mathbf{h}_{r+1} &= \bar{\mathbf{f}} \quad \text{with} \quad \mathcal{H} := \sum_{i=0}^l \underbrace{\mathbf{g}_{r+1}^T \mathbf{K}_i \mathbf{g}_{r+1}}_{=: k_i} \Delta_i, \quad \bar{\mathbf{f}} := (\mathbf{F} - \mathcal{A}(\mathbf{U}_r))^T \mathbf{g}_{r+1}, \end{aligned}$$

at which U_r is of course represented in its sum of dyadic products: $U_r = \sum_{i=1}^r g_i h_i^T$. As the stiffness matrix $K_i = K(\kappa_i)$ is linear with respect to its material κ_i , the coefficient matrix \mathcal{G} can be rewritten, which reduces the computational costs significantly:

$$\mathcal{G} = \sum_{i=0}^l d_i K(\kappa_i) = K(\sum_{i=0}^l d_i \kappa_i).$$

The coupled system 8 may be solved by an alternating iterative process, described in algorithm 1. This algorithm does not assure the mentioned optimal decomposition. Here the iterating vectors are simply normalised to keep them in bounds. The initial guess for the first rank-one update cannot be chosen as a zero vector. Otherwise the iterative process would stagnate. In this work the guess is chosen to be random. The first loop increments the rank, the second one performs the alternating iteration to compute the next rank-one update.

Algorithm 1 Variational Low-Rank approach with successive rank-one update.

```

1:  $\mathbf{H} \leftarrow \emptyset, \quad \mathbf{G} \leftarrow \emptyset$ 
2: while not accurate enough do
3:    $h \leftarrow \text{rand}, \quad g \leftarrow \text{init}$ 
4:   while not accurate enough do
5:      $h \leftarrow \text{normalise } h$ 
6:      $g \leftarrow \text{solve } \mathcal{G} g = \mathbf{f}$ 
7:      $g \leftarrow \text{normalise } g$ 
8:      $h \leftarrow \text{solve } \mathcal{H} h = \bar{\mathbf{f}}$ 
9:   end while
10:   $\mathbf{G} \leftarrow [\mathbf{G}, g]$ 
11:   $\mathbf{H} \leftarrow [\mathbf{H}, h]$ 
12: end while
```

Although each rank-one update is on its own the optimal one concerning the resulting energy, this algorithm computes a suboptimal Low-Rank representation of the solution, i.e U_r is not the minimiser of the energy with respect to all rank r matrices. In order to get the optimal rank r approximation another rank-one update scheme can be used, see algorithm 2.

The computations of the minimiser in algorithm 2 can be done by applying algorithm 1 to the reduced operators

$$\mathcal{A}_G := \sum_{i=0}^l G^T K_i G H^T \Delta_i = G^T F \quad \Longleftrightarrow \quad \mathcal{A}_G(H) = G^T F$$

resp.

$$\mathcal{A}_H := \sum_{i=0}^l K_i G H^T \Delta_i H = F H \quad \Longleftrightarrow \quad \mathcal{A}_H(G) = F H.$$

The initialisation for the next rank update is done by concatenating the zero column vector $\mathbf{0}$.

Algorithm 2 Variational Low-Rank approach with successive iterated rank-one update.

```

1:  $\mathbf{H} \leftarrow \emptyset, \quad \mathbf{G} \leftarrow \emptyset$ 
2: while not accurate enough do
3:    $\mathbf{G} \leftarrow [\mathbf{G}, \mathbf{0}]$ 
4:    $\mathbf{H} \leftarrow [\mathbf{H}, \mathbf{0}]$ 
5:   while not accurate enough do
6:      $v, g \leftarrow \text{minimiser } \mathcal{E}((\mathbf{G} + vg^T)\mathbf{H}^T)$ 
7:      $\mathbf{G} \leftarrow \mathbf{G} + vg^T$ 
8:      $w, h \leftarrow \text{minimiser } \mathcal{E}(\mathbf{G}(\mathbf{H} + wh^T)^T)$ 
9:      $\mathbf{H} \leftarrow \mathbf{H} + wh^T$ 
10:  end while
11: end while
  
```

A Posteriori Stochastic Solution Space Adaption in VLR-SR1U

The VLR-SR1U scheme motivates to develop advanced techniques to choose adaptively the solution space. In this work a simple a posteriori adaptive technique is introduced to select only relevant stochastic basis functions from a pool of stochastic basis functions. It is referred to as the *A Posteriori Stochastic Ansatz Space Adaption (APSASA)*. This technique is embedded in VLR-SR1U.

The main idea is derived from the consideration of the residual as an error indicator. The residual \mathbf{R} of the fully discretised groundwater flow problem (see equation 2) is given by

$$(9) \quad \mathbf{R} := \mathbf{F} - \sum_{i=0}^l \mathbf{K}_i \mathbf{U} \Delta_i.$$

The stochastic basis functions $\{\psi_\alpha\}_{\alpha \in \mathcal{I}^c}$ ($|\{\psi_\alpha\}_{\alpha \in \mathcal{I}^c}| = N_s$) are proposed to be extended by additional ones $\{\psi_{\alpha^+}\}_{\alpha^+ \in \mathcal{I}^{c^+}}$ ($|\{\psi_{\alpha^+}\}_{\alpha^+ \in \mathcal{I}^{c^+}}| = N_s^+$) without loosing their already used order. The idea now is to get an estimation of the influence of these new basis functions onto the solution and consequently to get an answer to the question, if these basis functions are relevant. Expanding each stochastic matrix Δ_i in that way leads to a resulting matrix

$$\Delta_i^\oplus := \left(\begin{array}{c|c} \Delta_i & \Delta_i^\triangleleft \\ \hline \Delta_i^\triangleright & \Delta_i^+ \end{array} \right).$$

The matrix Δ_i^+ only captures the additional basis functions, and the matrices Δ_i^\triangleleft and $\Delta_i^\triangleright = (\Delta_i^\triangleleft)^T$ capture the coupling between the original and the additional basis functions. These new matrices are declared by $[\Delta_i^+]_{\alpha^+, \beta^+} := \sum_{\gamma \in \mathcal{I}^c} \sqrt{\lambda_i} \xi_{i, \gamma} [\Delta_\gamma]_{\alpha^+, \beta^+}$ and $[\Delta_i^\triangleleft]_{\alpha^+, \beta} := \sum_{\gamma \in \mathcal{I}^c} \sqrt{\lambda_i} \xi_{i, \gamma} [\Delta_\gamma]_{\alpha^+, \beta}$. By using matrix Δ_i^\oplus another residual can be computed taking into account also the additional basis functions:

$$\mathbf{R}^\oplus := \mathbf{F}^\oplus - \sum_{i=0}^l \mathbf{K}_i \mathbf{U}^\oplus \Delta_i^\oplus.$$

U^\oplus means simply to resize U and to set the coefficients for the added basis functions to zero: $U^\oplus := [U, \mathbf{0}]$ with a N_x -by- N_s^+ zero matrix $\mathbf{0}$. F^\oplus is the concatenation of F and the right-hand side (RHS) F^+ concerning the added basis functions: $F^\oplus := [F, F^+]$. However the zero extension of U means to ignore automatically Δ_i^\triangleright and Δ_i^+ . Without this apparent redundancy the computationally more reasonable residual becomes

$$R^\oplus := F^\oplus - \sum_{i=0}^l K_i U \Delta_i^\oplus \quad \text{with} \quad \Delta_i^\oplus := [\Delta_i, \Delta_i^\triangleleft].$$

R^\oplus is a composition $R^\oplus = [R, R^+]$, where R is the original residual of equation 9. R^+ is the residual defined by the additional basis functions: $R^+ := F^+ - \sum_{i=0}^l K_i U \Delta_i^\triangleleft$. The residual composition R^\oplus may be used primarily to interpret the rating of the additional basis functions regarding the accuracy of the solution. However there is an interplay between the two single residuals. The case $\|R\| > \|R^+\|$ (with a suitable matrix norm $\|\cdot\|$) may identify, that the VLR-SR1U need to iterate more inside the current rank to reach a more reasonable accuracy before adapting the stochastic solution space to more basis functions. In contrast $\|R\| < \|R^+\|$ may identify, that the chosen additional basis functions would result in a better accuracy of the solution.

Numerical Experiments

The numerical behaviour of the VLR-SR1U algorithm and its extension to allow an adaptive construction of the solution space is demonstrated by approximating the solution of the mentioned stationary groundwater flow problem on a rectangular domain (see figure 1). Essential boundary conditions are applied on the left and right boundaries, natural conditions equal zero anywhere else. The source term is zero. The parameter κ is assumed to be lognormal distributed. The KLE of κ is truncated at five terms (the expected value excluded, that means $m = 5$). The maximum order of the PC basis functions of the solution is set to 4.

Table 1 shows the L_2 norm of the residual over the specific rank and the process of the energy minimisation along the successive rank-one updates of the VLR-SR1U algorithm. The corresponding number of iterations for each rank-one update are presented in figure 2. The break criterion inside a rank update was chosen by the relative error bound 10^{-6} and a maximum number of iterations of 100. In the cases, in which the maximum number of iterations was reached, the estimated relative error was lower than 10^{-5} .

The convergence rate of the VLR-SR1U algorithm is demonstrated at several statistical moments of two different kinds of functions onto the solution field, see table 2. The first function calculates the arithmetic mean at the entire geometrical domain. The second function calculates the arithmetic mean at the vertical middle of the geometrical domain. The convergence rate for the latter function is slightly worse, as the variance of the solution has its highest values at the considered vertical location. The evaluation of these functions onto the approximated solution field of the VLR-SR1U algorithm was done by Monte-Carlo integration with 100 million sample-points. The reference for the computation of the relative error was got by a SSFEM with a direct solver and a MC integration with 1 billion sample-points.

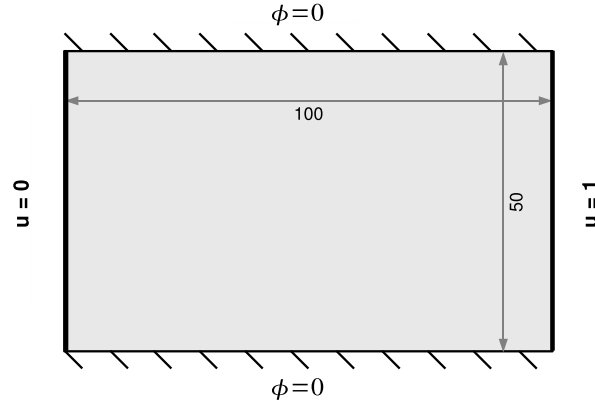


Figure 1: The rectangular domain of the considered groundwater flow problem with deterministic, heterogeneous essential conditions on the left and right boundary and natural condition anywhere else. The source term is zero.

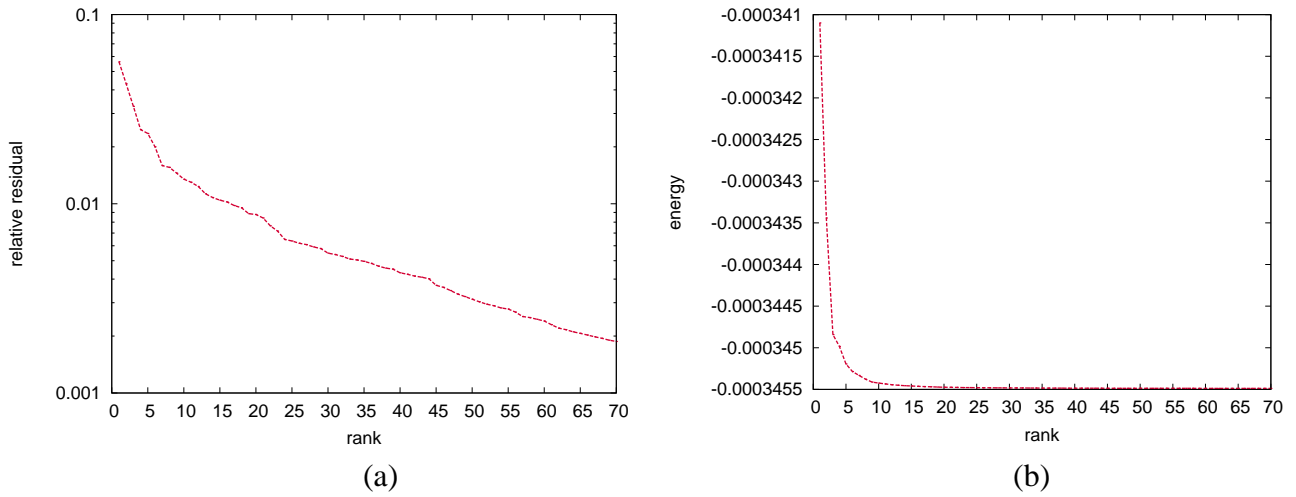


Table 1: Plot (a) shows the L_2 norm of the residual over the corresponding rank. Plot (b) shows the current expectation of the energy over the corresponding rank.

A stochastic solution space adaption inside the VLR-SR1U algorithm is pointed up in table 3. The adaption was performed for an approximation of rank 5.

Summary

We presented two Low-Rank algorithms based on the SSFEM with successive rank-one updates. Contrary to the second algorithm the first one does not necessarily provide an optimal decomposition regarding the minimum energy at a given rank. The algorithms are extended by an adaptive

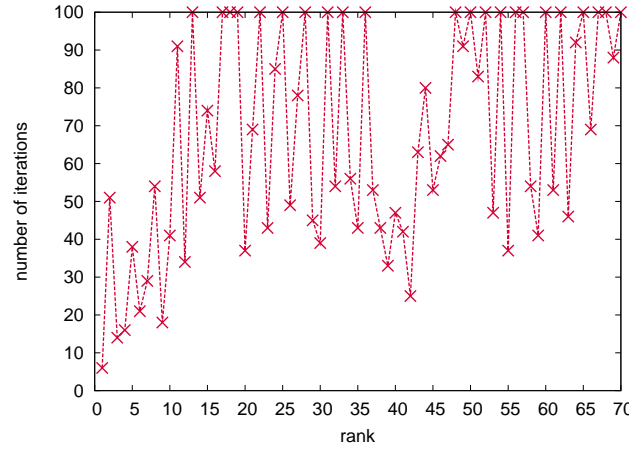


Figure 2: Number of iterations per rank update in VLR-SR1U. Break criterion is set to the L_2 norm of the residual $\leq 10^{-6}$ or maximum number of iterations 100. Some rank updates reached this maximum number. In all these cases the mentioned L_2 norm was below $\leq 10^{-5}$.

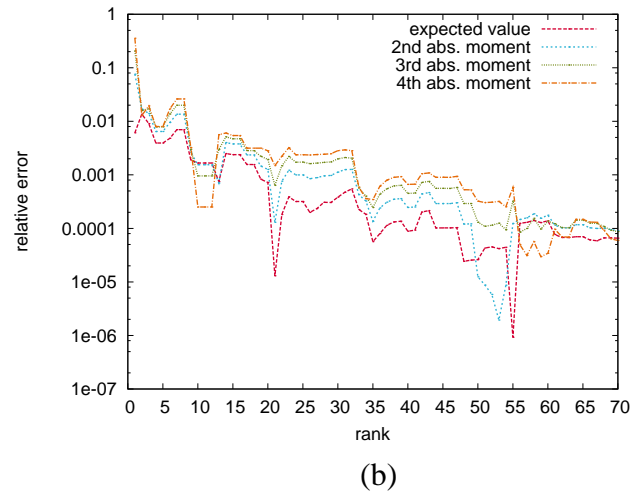
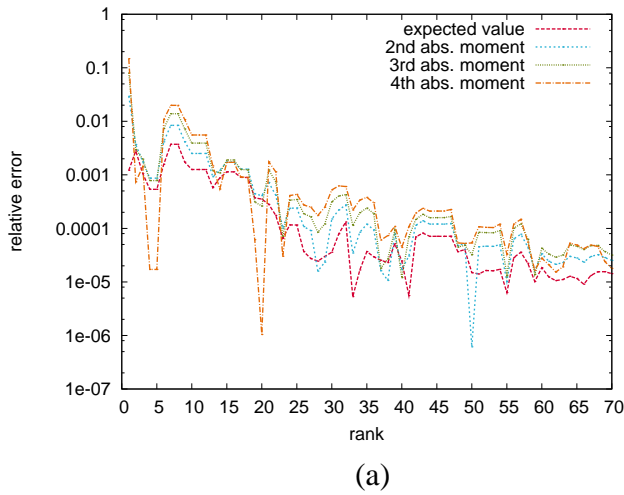


Table 2: Convergence rates of pure VLR-SR1U for the arithmetic average of the specified moments. The arithmetic average is computed (a) for the entire geometrical domain and (b) for the vertical geometrical middle of the rectangular domain. The relative error is plotted over the rank. The reference solution is taken from a SSFEM using a direct solver.

technique to construct the solution space a posteriori. In the latter case the residual is used to indicate, which stochastic degrees of freedom are the most promising ones for representing the solution. First numerical experiments show promise. However an adjustment is required.

	N_s	1 st	2 nd	3 rd	4 th
without APSASA	126	0.5000	0.2570	0.1355	0.0731
with APSASA	43	0.5003	0.2575	0.1360	0.0736

Table 3: Comparison between VLR-SRIU with and without solution space adaption (APSASA). N_s is the number of stochastic degrees of freedom. The expected value (“1st”) till to the fourth absolute moment (“4th”) of the arithmetic mean over the entire geometrical domain are given.

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